Star-quantization of an infinite wall

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Abstract: In deformation quantization (a.k.a. the Wigner-Weyl-Moyal formulation of quantum mechanics), we consider a single quantum particle moving freely in one dimension, except for the presence of one infinite potential wall. Dias and Prata pointed out that, surprisingly, its stationary-state Wigner function does not obey the naive equation of motion, i.e. the naive stargenvalue ($\star$-genvalue) equation. We review our recent work on this problem, that treats the infinite wall as the limit of a Liouville potential. Also included are some new results: (i) we show explicitly that the Wigner-Weyl transform of the usual density matrix is the physical solution, (ii) we prove that an effective-mass treatment of the problem is equivalent to the Liouville one, and (iii) we point out that self-adjointness of the operator Hamiltonian requires a boundary potential, but one different from that proposed by Dias and Prata.

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1. Introduction

Deformation quantization is also known as the Wigner-Weyl-Moyal formulation of quantum mechanics, and by other names.[1] We'll refer to it here as star-quantization. In it, as in classical mechanics, observables are realized as ordinary functions (and distributions) on phase space. They are multiplied, however, using a non-commutative, associative product, known as the star product ($\star$-product).

Star-quantization can be understood as the Wigner-Weyl transform of the quantum dynamics of the density matrix. On the other hand, it is an autonomous way of doing quantum mechanics. Quantum systems should therefore be treatable in it, without reference to operators and wave functions, or to path integrals, or to any other quantum formulation. That is, physical systems should be star-quantizable.

This note is concerned with the star-quantization of a very simple system, one particle moving freely along the negative x-axis, in the presence of an infinite potential wall at $x = 0$. Naive star-quantization does not work for it [2]. We would like to understand why it fails, and how the problem can be fixed.

Our considerations will be restricted to stationary states of the system. As emphasized in [3], where several examples were worked out, such stationary states are described by time-independent Wigner

[1] For an elementary review, see [1], which cites several more advanced reviews.

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functions that can be found as solutions of the so-called $\star$-genvalue equations.

We first introduce the $\star$-genvalue equations in section 2, and solve them for the Wigner function of a free particle moving on the entire x-axis. In the following section, the original problem [2], occurring when an infinite barrier is present at $x = 0$, is described. In section 4, we review our treatment [4] of the star-quantization of an infinite wall as the limit of an exponential potential. An alternative to the $\star$-genvalue equation was found that can be treated in the naive way: it can be solved first, and then the boundary conditions can be imposed later, to yield the physical Wigner function. In section 5, we note that the system can be treated using an effective mass. Interestingly, however, we show that the corresponding $\star$-genvalue equations are equivalent to those for the exponential potential. The ad hoc resolution of the problem proposed by Dias and Prata [2] (see also [5, 6]) is then described, in section 6. We have found in operator quantum mechanics a motivation for a result similar in form to, but in conflict with theirs. This is sketched in the same section 6. In [7], we plan to work out further consequences in star-quantization of this observation.

2. Free particle: $\star$-genvalue equation & Wigner-Weyl transform

Consider a single particle moving on the x-axis, so that its phase space is $\mathbb{R}^2$, with coordinates x, p. In star-quantization, the Wigner function encodes all observable information about the quantum state. Stationary states are described by time-independent Wigner functions $\rho(x,p)$, that can be found as solutions to the so-called $\star$-genvalue equations

$$H \star \rho \;=\; \rho \star H \;= E\rho \;\; . \tag{1}$$

Here, $H = H(x,p)$ is the classical Hamiltonian, E is the energy, and the Grönewold-Moyal $\star$-product is defined by

$$f(x,p) \star g(x,p) \;=\; \exp\left[i\hbar\left(\partial_x\partial_{p'} - \partial_p\partial_{x'}\right)/2\right]\, f(x,p)\, g(x',p')\big|_{(x',p')=(x,p)} \; . \tag{2}$$

Real solutions of these equations will describe quantum states, but they will be mixed states, in general. In this work, we will only consider pure states, whose Wigner functions obey the additional $\star$-projection condition

$$\rho_i \star \rho_j \;=\; \delta_{ij}\, \rho_j/h \; , \;\; \text{or} \;\;\; \rho_\alpha \star \rho_\beta \;\propto\; \delta(\alpha-\beta)\, \rho_\beta/h \; , \tag{3}$$

for states labelled by discrete parameters $i, j, \ldots$, or for non-normalizable states labelled by continuous parameters $\alpha, \beta, \ldots$, respectively.

To illustrate, let us first consider a free particle (see the Appendix of [4]). The Hamiltonian is $H = p^2$, if we set $2m = 1$ for simplicity. The $\star$-genvalue equations (1) then reduce to

$$(p - i\hbar\partial_x/2)^2\rho(x,p) \;=\; k^2\rho(x,p) \; , \tag{4}$$

where we have put $E = k^2$, and we will work henceforth with $\hbar = 1$. The imaginary part of this equation is $p\,\partial_x\rho \;=\; 0$, so that when $p \neq 0$, $\partial_x\rho = 0$, but not when $p = 0$. This leads to the ansatz

$$\rho(x,p) \;=\; f(p) + \delta(p)\, g(x) \; . \tag{5}$$

In the real part of (4), $(p^2 - \partial_x^2/4)\,\rho \;=\; k^2\,\rho$, it yields

$$(p^2 - k^2)\, f(p) \;-\; \delta(p)(k^2 + \partial_x^2/4)\, g(x) \;=\; 0 \; . \tag{6}$$

Considering $p = 0$ gives

$$g(x) \;=\; b\exp(2ikx) \;+\; b^*\exp(-2ikx) \; , \tag{7}$$

where $\rho = \rho^*$ has been imposed. Then (6) reduces to $(p^2 - k^2)\, f(p) = 0$, solved by

$$f(p) \;=\; a_+\delta(p-k) \;+\; a_-\delta(p+k)\;, \tag{8}$$

with $a_\pm$ arbitrary real constants. The general result is therefore

$$\rho \;=\; \delta(p)\left\{\, b\exp(2ikx) \;+\; b^*\exp(-2ikx)\,\right\} \;+\; a_+\delta(p-k) \;+\; a_-\delta(p+k)\;. \tag{9}$$

To restrict to pure-state Wigner functions, we impose $\rho\star\rho\;\propto\;\delta(0)\,\rho$, a special case of (3). We find the constraint

$$|b|^2 \;=\; a_+a_- \;\;\Rightarrow\;\; b \;=\; \sqrt{a_+a_-}\,e^{i\phi}\;,\; \phi\in\mathbb{R}\,. \tag{10}$$

The general pure-state solution to the free-particle $\star$-genvalue equation (4) is therefore

$$\rho \;=\; a_+\delta(p-k) \;\;+\;\; a_-\delta(p+k) \;+\;\; 2\sqrt{a_+a_-}\;\delta(p)\,\cos\big(2kx+\phi\big)\;. \tag{11}$$

On the other hand, the Wigner function can be calculated as the (normalized) Wigner-Weyl transform of the density matrix $|\psi\rangle\langle\psi|$, built from the known wave functions:

$$\rho[\psi] \;:=\; \frac{1}{\pi}\int_{-\infty}^{\infty} dy\, e^{-2ipy}\,\psi(x+y)\,\psi^*(x-y)\;. \tag{12}$$

We denote it as $\rho[\psi]$ here to emphasize that it is calculated from known input wave functions, and so is not a result of working within the star-quantization formulation. With the pure-state wave function $\psi \;=\; \alpha_+e^{ikx} \;+\; \alpha_-e^{-ikx}$, eqn. (12) yields

$$\rho[\psi] \;=\; |\alpha_+|^2\delta(p-k) \;+\; |\alpha_-|^2\delta(p+k) \;+\; \delta(p)\big\{\alpha_+^*\alpha_-e^{-2ikx} \;+\; \alpha_+\alpha_-^*e^{2ikx}\big\}\;. \tag{13}$$

Comparing (13) with (11) reveals a one-to-one correspondence. All is well for the free particle.

3. Infinite wall: $\star$-genvalue equation vs Wigner-Weyl transform

Now consider the Hamiltonian $H = p^2 + V(x)$, with potential energy

$$V(x) \;=\; \begin{cases} 0\,, & x<0\,;\\ \infty\,, & x>0\,. \end{cases} \tag{14}$$

We first work out the Wigner-Weyl transform of the known Schrödinger wave functions

$$\psi(x) = \theta(-x)\,\sin(kx)\;. \tag{15}$$

Here $\theta(x)$ denotes the Heaviside step function. From (12) we find

$$\rho[\psi] \;\propto\; \theta(-x)\,\bar\rho(x,p)\;, \tag{16}$$

with

$$\bar\rho(x,p) \;=\; \frac{\sin[2x(p+k)]}{2(p+k)} \;+\; \frac{\sin[2x(p-k)]}{2(p-k)} \;-\; 2\cos(2xk)\,\frac{\sin(2xp)}{2p}\;. \tag{17}$$

This can be obtained from a special case of the free-particle Wigner function (11) by the replacement $\delta(p-p_0)\;\to\;\sin[2x(p-p_0)]/[2(p-p_0)]$. The latter vanishes at $x=0$, so that $\bar\rho(0,p)=0$, and becomes the former when $x\to-\infty$, so that a free-particle result is found far from the infinite wall.

We will show in the following section that (16, 17) describe the physical Wigner function, the one that should be found in the star-quantization of an infinite wall.

To solve the $\star$-genvalue equations (1) with the Hamiltonian determined by (14), we can try to follow the Schrödinger treatment of this system, by restricting to $x<0$, and then imposing the boundary condition $\rho(0,p)=0$. For $x<0$, the $\star$-genvalue equation is that of a free particle, however, eqn. (4). The problem is that the Wigner function given by (16, 17) does not satisfy this equation.

4. Infinite barrier as the limit of an exponential potential

To study this problem, we treated the Hamiltonian of the previous section as the $\alpha \to \infty$ limit of

$$H_\alpha = p^2 + e^{2\alpha x} \ . \tag{18}$$

Star-quantization of this system had already been carried out at $\alpha = 1$, in [3]. The α-dependence was easily reinstated. The physical Wigner function is given by (cf. eqn. (98) of [3])

$$\begin{aligned}\rho_\alpha \quad \propto \quad & \int_C ds \left[\tfrac{e^{4\alpha x}}{(2\alpha)^4}\right]^s \Gamma\Big(\tfrac{i}{2\alpha}(p-k)-s\Big)\,\Gamma\Big(\tfrac{i}{2\alpha}(p+k)-s\Big) \\ & \times \Gamma\Big(\tfrac{-i}{2\alpha}(p-k)-s\Big)\,\Gamma\Big(\tfrac{-i}{2\alpha}(p+k)-s\Big) \ . \end{aligned} \tag{19}$$

The contour C in the s plane runs from $-i\infty$ to $+i\infty$, just to the left of the four poles on the imaginary s axis at $\pm\frac{i}{2\alpha}(p \pm' k)$. The right-hand side of (19) is the Mellin-Barnes type integral definition of the Meijer G-function (see §5.3. of [8]), so

$$\rho_\alpha \propto \ G^{40}_{04}\left(\frac{e^{4\alpha x}}{(2\alpha)^4} \middle| \frac{i(p-k)}{2\alpha}, \frac{i(p+k)}{2\alpha}, \frac{-i(p-k)}{2\alpha}, \frac{-i(p+k)}{2\alpha} \right) \ . \tag{20}$$

First, consider the $\alpha \to \infty$ limit of the Wigner function. For $x > 0$, $w = e^{4\alpha x}/(2\alpha)^4 \to \infty$, but $G^{40}_{04}(w|\cdot) \to 0$ exponentially, according to the asymptotics described in §5.4.1 of [8].

For $x < 0$, the contour C can be closed such that all 4 poles on the imaginary s-axis, at $s = i(\pm p \pm' k)/2\alpha$, are surrounded. First note that

$$\lim_{\alpha\to\infty} (2\alpha)^{-2i(\pm p \pm' k)/\alpha} \ = \ 1 \ . \tag{21}$$

We can now apply the residue theorem and use $\Gamma(z) = \Gamma(1+z)/z$, to find $\rho_\alpha(x,p)$ goes as

$$\begin{aligned} & e^{2ix(p-k)}/(-2ik)2(ip-ik)(2ip) \ + \ e^{2ix(p+k)}/(2ik)(2ip)2(ip+ik) \\ & + e^{-2ix(p-k)}/2(-ip+ik)(-2ip)(2ik) \ + \ e^{-2ix(p+k)}/(-2ip)2(-ip-ik)(-2ik) \ , \end{aligned} \tag{22}$$

as $\alpha \to \infty$, up to a factor depending on α, but independent of x. But this is proportional to

$$\begin{aligned} & e^{2ix(p-k)} \left(\tfrac{1}{kp} - \tfrac{1}{k(p-k)}\right) \ + \ e^{2ix(p+k)} \left(\tfrac{1}{kp} - \tfrac{1}{k(p+k)}\right) \\ & - e^{-2ix(p-k)} \left(\tfrac{1}{kp} - \tfrac{1}{k(p-k)}\right) \ - \ e^{-2ix(p+k)} \left(\tfrac{1}{kp} - \tfrac{1}{k(p+k)}\right) \ . \end{aligned} \tag{23}$$

Comparing with (17), we see that for $x < 0$, we have shown that $\lim_{\alpha\to\infty} \rho_\alpha \ \propto \ \bar\rho$.

Combining the results for $x < 0$ and $x > 0$, we have that $\lim_{\alpha\to\infty} \rho_\alpha \ \propto \ \theta(-x)\,\bar\rho$. That is, the limit of the Wigner function for the exponential potential is $\theta(-x)\,\bar\rho$, showing that (16) and (17) describe the physical Wigner function for the infinite potential wall. The authors of [2], e.g., made this assumption.

Our goal is to find a dynamical equation that this physical Wigner function satisfies, instead of the $\star$-genvalue equation, which it does not. The new equation [4] can then be used to solve for the physical Wigner function, i.e., the new equation can be used to carry out a true star-quantization of the infinite potential wall.

Following [3], we see that (18) yields a $\star$-genvalue equation $H_\alpha \star \rho_\alpha \ = \ k^2\,\rho_\alpha$ with imaginary and real parts

$$\begin{aligned} e^{-2\alpha x}\,\partial_x \rho_\alpha(x,p) \ &= -\ \tfrac{i}{2p}\left[\rho_\alpha(x,p+i\alpha) - \rho_\alpha(x,p-i\alpha)\right] \ , \\ e^{-2\alpha x}\left(p^2 - k^2 - \tfrac{1}{4}\,\partial_x^2\right)\rho_\alpha(x,p) \ + \ \tfrac{1}{2}\left[\rho_\alpha(x,p+i\alpha) + \rho_\alpha(x,p-i\alpha)\right] \ &= \ 0 \ , \end{aligned} \tag{24}$$

respectively. These two equations can be recombined into a difference equation:[2]

$$0 \;=\; (p^2-k^2)\rho_\alpha(x,p)+\frac{1}{p}\left(\frac{e^{2\alpha x}}{4}\right)^2\left[\frac{\rho_\alpha(x,p+2i\alpha)-\rho_\alpha(x,p)}{p+i\alpha}+\frac{\rho_\alpha(x,p-2i\alpha)-\rho_\alpha(x,p)}{p-i\alpha}\right]$$
$$-\frac{ie^{2\alpha x}}{4p}\left[\rho_\alpha(x,p+i\alpha)-\rho_\alpha(x,p-i\alpha)\right]+\frac{e^{2\alpha x}}{2}\left[\rho_\alpha(x,p+i\alpha)+\rho_\alpha(x,p-i\alpha)\right]\ . \tag{25}$$

In [4], we showed that $\rho_\alpha(x,p\pm i\alpha),\ \rho_\alpha(x,p\pm 2i\alpha)$ could be traded for $\partial_x^n\rho_\alpha(x,p),\ n=1,2,3,4$, to arrive at a differential equation, with a simple $\alpha\to\infty$ limit,

$$\partial_x^4\rho(x,p)/16\ +\ (p^2+k^2)\,\partial_x^2\,\rho(x,p)/2\ +\ (p^4-2k^2p+k^4)\,\rho(x,p)\ =\ 0\ , \tag{26}$$

valid for $x<0$. Recalling that $E=:k^2$, the new equation can be rewritten as

$$(p^2-E)\star\rho\star(p^2-E)\ =\ 0\ . \tag{27}$$

It is easily verified that $\bar\rho$ of (17) satisfies the new equation. In [4] it was also shown that the new equation applies to other systems built from infinite walls or wells: the infinite square well and the delta-function well. Furthermore, it was shown how an additional, non-singular potential could be included in the framework.

The proposal made in [4] was to star-quantize the infinite-wall system by solving the new equation, and then imposing the boundary conditions, much as for solutions of the Schrödinger equation. Some progress in this direction was made in [6].

5. Effective mass treatment

Let us mention another possible approach. It is clear that the free Hamiltonian $H=p^2$ encodes nothing of the dynamics of the infinite potential wall at $x=0$. In the Schrödinger treatment, imposing the boundary conditions suffices to yield the required physics, but not in star-quantization. Can the dynamics of the wall be described by a modified Hamiltonian?

One could try to incorporate the dynamics in the kinematics, by assigning to the particle an effective mass that blows up for $x>0$. In the spirit of the last section, such a Hamiltonian can also be considered as a limit:

$$H'_{\rm eff}\ :=\ \theta(-x)\,p^2\ =\ \lim_{\alpha\to\infty}\ H'_{\text{eff},\,\alpha}\ :=\ \lim_{\alpha\to\infty}\ \left(1+e^{2\alpha x}\right)^{-1}\,p^2\ \ . \tag{28}$$

We will now show that

$$H'_{\text{eff},\,\alpha}(x',p)\star\rho'_{\rm eff}(x',p)\ =\ k^2\,\rho'_{\rm eff}(x',p) \tag{29}$$

is equivalent to the $\star$-genvalue equation with Hamiltonian H_α of (18), already considered.

Using (2), one can show that (29) reduces to

$$(p-i\partial_{x'}/2)^2\,\rho'_{\text{eff},\,\alpha}(x',p)\ =\ k^2\,(1+e^{2\alpha x'+i\alpha\partial_p})\,\rho'_{\text{eff},\,\alpha}(x',p)\ . \tag{30}$$

Writing $x'\ =\ x\ +\ \log(-k^2)/(2\alpha)$ yields

$$(p-i\partial_x/2)^2\,\rho_\alpha(x,p)\ =\ (k^2-e^{2\alpha x+i\alpha\partial_p})\,\rho_\alpha(x,p)\ , \tag{31}$$

however, where we put $\rho_\alpha(x,p):=\rho'_{\text{eff},\,\alpha}(x',p)$. The transformed equation is just $H_\alpha(x,p)\star\rho_\alpha(x,p)\ =\ k^2\rho_\alpha(x,p)$, the $\star$-genvalue equation for (18). Since $x'-x\to 0$ in the $\alpha\to\infty$ limit, (29) must lead to the same eqn. (27) we already found above.

[2] At $\alpha=1$, this is a slight correction of eqn. (104) of [3].

6. Self-adjoint extensions and boundary potentials

Let us reconsider the operator treatment of the system, to try to understand why pure star-quantization fails. Perhaps the problem will turn out to be the Wigner-Weyl transform of one already present in the operator formulation.

A self-adjoint Hamiltonian $\hat{H}$ will have a spectral decomposition, $\hat{H} = \sum_{E'} |E'\rangle\langle E'|$, roughly speaking. Then for a pure-state density matrix $\hat{\rho} = |E\rangle\langle E|$ built from the stationary energy eigenstate $|E\rangle$, we necessarily have $\hat{H}\hat{\rho} = \hat{\rho}\hat{H} = E\hat{\rho}$. If the Wigner-Weyl transform $\mathcal{W}$ works, these become the $\star$-genvalue equations (1).

The key realization is that the free Hamiltonian operator $\hat{H} := \hat{p}^2$ is not self-adjoint on the negative x-axis, even if it is Hermitian (see [9], e.g., and references therein). We believe that this is the root cause of at least part of the problem encountered with naive star-quantization of the infinite wall.

The free Hamiltonian $\hat{H}$ does have self-adjoint extensions, however, as can be determined by calculating its von Neumann deficiency indices. The extensions amount to including a point interaction at $x = 0$. The role of the point interaction is to enforce a (Robin) boundary condition on the Schrödinger wave function, involving a real length L:

$$\psi(0) \ + \ L\psi'(0) \ = \ 0 \quad (\psi' := d\psi/dx) \ . \tag{32}$$

It is easy to see that such a potential takes the form $V_L(x) = \delta(x) \ - \ L\delta'(x)$.

A specific interaction of this type was prescribed in an ad hoc way by Dias and Prata, for the boundary condition $\psi(0) = 0$. It is interesting to note, however, that their prescription was for a boundary potential proportional to $\delta'_-(x)$, a regularized version of $\delta'(x)$. Apparently, this contradicts the standard operator treatment, since the Dirichlet boundary condition corresponds to $L = 0$ in (32), which relates to $V_{L=0}(x) = \delta(x)$.

Clearly, the situation needs clarification. We hope to report further progress on this problem in [7].

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